Nonlinear evolution and stability of the heat flow in nanosystems: Beyond linear phonon hydrodynamics

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A heat-transport equation incorporating nonlocal and nonlinear contributions of the heat flux is derived in the framework of weakly nonlocal nonequilibrium thermodynamics. The motivation for these terms arises from applications to nanosystems, where strong gradients are found, due to the small distance over which changes in temperature and heat flux take place. This equation generalizes to the nonlinear domain previous equations used in the context of phonon hydrodynamics. Compatibility with second law of thermodynamics is investigated and a comparison with the thermomass model of heat transport is carried out. The analogy between the equations describing the heat flow problem and the hydrodynamic equations is shown and the stability of the heat flow is analyzed in a special case.

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I. INTRODUCTION

In the last decades, one-dimensional nanostructures (such as wires, rods, belts, and tubes) have drawn significant attention owing to their potential application in nanoelectronics, photonics, and energy-conversion devices.[1–5] The continuous reduction in the sizes in these devices brings up new questions concerning the analysis of heat transport. Several experiments or simulations on heat transport along these devices have obtained results that differ significantly from those predicted by the classical Fourier law.[4,6–9] In fact, as it has been widely demonstrated, nanosystems exhibit a strong size dependence of their electronic and optical properties.[10,11] Indeed, due to the small sizes of the systems, the gradients of the heat flux will be important (and therefore, their influence through nonlocal terms must be incorporated) as well as temperature gradients, acting as thermodynamic forces, whose nonlinear effects will be not negligible. It is, therefore, important to examine more deeply the influence of nonlocal and nonlinear effects, and generalized heat transport equations must be looked for.

From a microscopic point of view, a simple model illustrating relaxational and nonlocal effects in heat transport is the phonon gas hydrodynamics.[12] In such a framework, the solution of the linearized Boltzmann equation leads to the well-known Guyer-Krumhansl equation[13–15]

$$\tau_R \dot{q}_i + q_i = -\kappa\theta_{,i} + l^2(q_{i_{,kk}} + 2q_{k_{,ki}}), \tag{1}$$

with q_i, $i=(1,2,3)$, as the components of the heat flux, θ as the absolute nonequilibrium temperature, $l^2=(9/5)\chi\tau_N$ as the mean-free path of phonons, and $\chi=\kappa/c_v$ as the thermal diffusivity, being κ the bulk thermal conductivity and c_v the specific heat at constant volume. Moreover, τ_R and τ_N mean the relaxation times related to resistive and normal phonon scatterings,[15,16] respectively. The upper dot on q_i stands for the material time derivative, whose convective part will be discussed in Sec. IV.

Equation (1), whose macroscopic derivation can be obtained in the framework of weakly nonlocal nonequilibrium thermodynamics,[1,17] does not include nonlinear effects, since it has been derived under the hypothesis that the thermophysical quantities are constant. On the other hand, a nonlinear extension of Eq. (1) should account for two different types of phenomena. First of all, as heat conduction measurements in crystals show clearly, the material functions κ, c_v, τ_R, and τ_N are temperature dependent.[15,18–20] Moreover, in nanosystems, due to the small size of the heat conductor, small temperature differences could lead to high values of temperature gradient, and as a consequence nonlinear terms accounting for products of the temperature gradient or the heat flux must also be taken into consideration.

In the present paper we derive and discuss in detail a generalization of Eq. (1) which takes into account both the aforementioned effects. The difference with some previous approaches is the emphasis on the dynamical character of the heat flux (also assumed in Grad's approach to kinetic theory[1]) and on the analogies with hydrodynamical equations, the heat flux playing a role analogous to the velocity of a fluid, an approach which is of interest in the domain of the so-called phonon hydrodynamics.

The simplest nonlinear extension of Eq. (1) can be written as

$$\tau_R \dot{q}_i + q_i = -\kappa\theta_{,i} + l^2(q_{i_{,kk}} + 2q_{k_{,ki}}) + \mu q_k q_{k_{,i}}, \tag{2}$$

with μ as suitable material coefficient. For constant material functions, Eq. (2) has been derived in Refs. 21 and 22. Here we obtain the equation above from a more general model in which the thermophysical quantities depend on the temperature. The expression of μ will be determined on thermodynamical grounds.

In the following, we describe relaxational heat transfer in terms of a dynamical nonequilibrium temperature β, ruled by a suitable evolution equation, to be determined on purely thermodynamic grounds.[21–23] The essential idea of this approach is that the heat flux is given by

$$q_i = -\kappa \beta_{,i}. \tag{3}$$

According with the Fourier law, this formalism still assumes that heat flows in the opposite direction of the gradient of a potential function. However, in contrast with it, this potential is β rather than θ. The main differences between β and θ, and the consequence of Eq. (3) on the second-sound propagation have been pointed out in a recent paper by Jou *et al.*[24] Equation (3) is capable to reproduce different heat conduction regimes, depending on the evolution equation of β. Other ways to derive an equation such as Eq. (2) without direct use of the dynamical nonequilibrium temperature β are also possible, but we have preferred to use it in the line of our previous papers.[21,22]

In linear situations, namely, for constant material functions, the different thermodynamic regimes, such as parabolic and hyperbolic heat conduction,[25] as well as the energy equation in the phonon scattering model and the energy equation in the phonon-electron interaction model,[26] can all be connected with the dual-phase-lagging constitutive equation for heat conduction (also named Tzou equation[5,27]), relating the temperature gradient at a material point **x** and time $t+\tau_T$, to the heat flux vector at **x** and time $t+\tau_q$. The model proposed here cannot be incorporated in the Tzou equation since it allows both the relaxation times to depend on the temperature.

The present paper runs as follows. In Sec. II we derive the model equations and investigate their compatibility with second law of thermodynamics. In Sec. III, we derive a nonlinear extension of the Guyer-Krumhansl equation and point out the conditions under which Eqs. (1) and (2) can be recovered. In Sec. IV we compare the nonlocal nonlinear heat-transport equation proposed here with that proposed in the so-called thermomass model for heat transport.[28–30] In Sec. V we show that in particular situations our nonlinear transport equation takes a form similar to the classical Navier-Stokes equation of incompressible viscous hydrodynamics. To show that, in the context of phonon hydrodynamics we first define some characteristic quantities (i.e., the thermal analogous of the well-known dimensionless numbers used in hydrodynamics) related to the geometry of the system as well as to the characteristic time of the phenomenon and to the standard physical conditions under which it takes place. Then, we recover the hydrodynamic equations under suitable hypotheses on these numbers. We also consider an initial and boundary value problem for the heat flow and an initial perturbation of it, and point out in what conditions the flow is unstable under such a perturbation. In Sec. VI we summarize and discuss the results of the previous sections.

II. PHYSICAL MODEL

Nonlinear effects may be understood in two different ways: as a temperature dependence in the material functions or as the presence of nonlinear products of the temperature gradient (or the heat flux) in the transport equations. The effects of both these kinds of nonlinearities on second-sound propagation have been analyzed in Refs. 21 and 31. In the present section we postulate a suitable nonlocal and nonlinear evolution equation for β, implying a correspondent evolution equation for the heat flux, and assume that the material functions are temperature dependent, i.e., $\kappa=\kappa(\theta)$, $c_v=c_v(\theta)$, $\tau_R=\tau_R(\theta)$, and $\tau_N=\tau_N(\theta)$. Then, let us consider a rigid heat conductor whose thermodynamic state space is spanned by the specific internal energy e and the dynamical nonequilibrium temperature β, together with their first-order gradients, namely, $\mathcal{Z}=\{e;e_{,k};\beta;\beta_{,k}\}$. The motivation for the inclusion of the gradients of e and β as independent state-space variables rests on the description of nonlocal effects.

The state variable e is governed by the local balance of energy

$$\dot{e} = -q_{i_{,i}}, \tag{4}$$

with the heat flux given by the constitutive assumption in Eq. (3).

Moreover, let us suppose that β is ruled by the following evolution equation:

$$\dot{\beta} = -\frac{(\beta-\theta)}{\tau_R} - \frac{\chi}{\theta}\beta_{,i}\beta_{,i} + g(\theta)\beta_{,ii}, \tag{5}$$

where g is a suitable regular function of θ, whose form may be determined by second law of thermodynamics. The first term in the right-hand side of Eq. (5) describes the relaxation of β toward θ. If only this term is considered, the combination of Eqs. (4) and (5) leads to a purely relaxational generalization of the Fourier's equation, namely, Eq. (1) with $l=0$. Equation (5) explicitly models nonlocal effects through the first- and second-order spatial derivatives of β. It is the simplest extension of the evolution equation obtained in Ref. 22 [see Eq. (54) therein] since the nonlocal effects arising from $\beta_{,ik}$ have been taken into account only through its first invariant, i.e., through a linear term in $\beta_{,ii}$. Moreover, Eq. (5) is in accordance with the general theorems of representation for isotropic scalar functions depending on scalar, vector, and tensor variables.[32]

Before to proceed further, let us investigate the compatibility of the model represented by Eqs. (3)–(5) with second law of thermodynamics, under the hypothesis of temperature-dependent material functions. In the present case, the second law locally reads

$$\dot{s} + \Phi_{i_{,i}} \geq 0, \tag{6}$$

being s the entropy density, and Φ_i, the components of the entropy flux.[1]

To exploit inequality in Eq. (6) we use a generalization of the classical Liu procedure,[33] accounting for thermodynamic restrictions on the coefficients of higher-order derivatives.[34,35] Passing over the cumbersome algebraic manipulations (refer to Refs. 34 and 35 for a detailed illustration of such a procedure and to Ref. 22 for its application to heat transport), in what follows we point out the main results.

First of all, it turns out that the specific entropy s is nonlocal both with respect to e and β. Up to the second order in $e_{,i}$ and $\beta_{,i}$, a suitable form of s is

$$s(e;\beta;e_{,k};\beta_{,k}) = s_0(e) - \frac{1}{2}s_e(e;\beta)e_{,i}e_{,i} - \frac{1}{2}s_\beta(e;\beta)\beta_{,i}\beta_{,i}, \tag{7}$$

where $s_0(e)$ is the equilibrium part of the entropy while $s_e(e;\beta)$ and $s_\beta(e;\beta)$ are regular scalar functions. Although this expression is not the most general one, it is suggested by the general theorems of representation of isotropic scalar functions depending on scalar and vector variables.[32] Moreover it ensures that the principle of maximum entropy at the equilibrium is fulfilled, provided $s_e(e;\beta)$ and $s_\beta(e;\beta)$ are positive definite.[36]

Due to the classical definition of absolute nonequilibrium temperature,[37] namely, $\theta^{-1}=\partial s/\partial e$, we infer that $\theta=\theta(e;\beta;e_{,k};\beta_{,k})$, in general, is a truly nonequilibrium quantity, which is strongly influenced by nonlocal effects. Indeed, along with this result and the assumed dependence on θ of the material functions, one would observe that, in principle, κ, c_v, τ_R, and τ_N, would depend on the whole set of the state variables, too. However, since we did not find any dependence of the material functions on the gradients, either in the experimental observations on dielectric crystals,[15,18–20] or in those on silicon nanowires and carbon nanotubes,[4,6–9,38] in the next we will suppose they may only depend on e and β, whereas we let g to depend on the whole set of the state variables. In particular, the second-law forces g to be given by

$$g(\theta) = -\frac{\kappa}{\beta_{,k}\beta_{,k}}\frac{s_e(e;\beta)}{s_\beta(e;\beta)}e_{,i}\beta_{,i}. \tag{8}$$

Although by Eq. (8) the mathematical form of g appearing in Eq. (5) may be obtained easily, at this step its physical meaning is still unknown. The study of the nonlinear Guyer-Krumhansl equation in Sec. III will offer a mean to determine it.

Finally, our analysis is able to show (see Refs. 34 and 35 for explicit details) that the entropy flux may have a constitutive equation which is more complex than that postulated in rational thermodynamics,[37] namely, more complex than $\Phi_i=q_i/\theta$.

III. NONLINEAR GUYER-KRUMHANSL EQUATION

Starting from the theory of heat conduction with dynamical temperature β, in the present section we derive a nonlinear extension of the Guyer-Krumhansl equation. To achieve that task we have to calculate the time derivative of q_i, and its first- and second-order spatial derivatives. Indeed, due to the constitutive assumptions on the material functions, combination of Eqs. (3) and (4) yields

$$\dot{q}_i = -\kappa\dot{\beta}_{,i} - \frac{1}{c_v}\frac{\partial \ln \kappa}{\partial \theta}q_{k_{,k}}q_i. \tag{9}$$

Analogously, it is possible to obtain the following expression for the gradient of the heat flux:

$$q_{k_{,i}} = -\kappa\beta_{,ki} + \frac{\partial \ln \kappa}{\partial \theta}q_k\theta_{,i}. \tag{10}$$

In order to simplify our analysis, in what follows we will consider each time and/or space derivative as a first-order term and will neglect third-order terms. Under the assumptions above, the second-order gradients of q_i can be calculated keeping the algebraic manipulations down to a reasonable level and still retaining sufficient generality.

Then, combining the gradient extension of Eq. (5) with the obtained expressions for the second-order gradients of q_i, and still disregarding third-order terms, it is possible to obtain the following nonlinear extension of the Guyer-Krumhansl equation:

$$\begin{aligned}\tau_R\dot{q}_i + &\left[1 + \frac{\tau_R}{c_v}\frac{\partial \ln \kappa}{\partial \theta}\left(1 + \frac{g}{3}\frac{F}{\kappa}\right)q_{k_{,k}}\right]q_i \\ &= -\kappa\left\{1 + (\beta-\theta)\frac{\partial \ln \tau_R}{\partial \theta} - \frac{\tau_R}{\kappa}\left[\frac{\partial g}{\partial \theta} - \frac{2}{3}g\frac{\partial \ln \kappa}{\partial \theta}\right]q_{k_{,k}}\right\}\theta_{,i} \\ &\quad + g\frac{\tau_R}{3}(q_{i_{,kk}} + 2q_{k_{,ki}}) + 2\frac{\tau_R}{c_v\theta}\left(1 - gF\frac{\theta}{\kappa}\frac{\partial \ln \kappa}{\partial \theta}\right)q_kq_{k_{,i}},\end{aligned} \tag{11}$$

wherein the function $F(\theta)$ is defined as $F=(s_\beta g)/(s_e\kappa)$.

In order to recover Eq. (2) as a special case of Eq. (11), i.e., when in it the terms in $\partial/\partial\theta$ are negligible, we make the following identifications:

$$g(\theta) = \frac{27}{5}\chi\frac{\tau_N}{\tau_R}, \tag{12a}$$

$$\mu = 2\frac{\tau_R}{c_v\theta}. \tag{12b}$$

Equation (12b) allows us to identify the coefficient μ of the nonlinear term in Eq. (2) in terms of physically well-known quantities. Note that our model is nonlinear even for constant material functions, since, in this case, Eq. (11) does not reduce to Eq. (1), but contains a further nonlinear term in $q_kq_{k_{,i}}$ whose physical relevance will be discussed later. Moreover, a comparison between Eqs. (2) and (11) without nonlinear terms, allows us to identify $g(\theta)$ as the ratio l^2/τ_R, once Eq. (12a) holds.

In closing this section, let us give a further comment about Eq. (11). In the first term of its right-hand side a dynamical heat conductivity, depending on $\beta-\theta$ (namely, on $\dot{\beta}$), appears. Close to the equilibrium of β, i.e., for $\beta-\theta$ negligible with respect to the other terms entering the dynamical heat conductivity, such a function depends on θ only.

IV. COMPARISON WITH THE THERMOMASS MODEL OF HEAT TRANSPORT

The central topic of interest of the present paper is the nonlinear and nonlocal transport equation for the heat flux. Thus, it is of interest to compare our approach with other proposals searching also for such an equation. In particular, in the present section we will compare our model with the so-called thermomass model of heat transport,[28–30] which also aims to propose a hydrodynamic-like description of the heat flux. In this approach, an effective mass density (i.e., the so-called thermomass density) ρ^h is attributed to the phonon gas. It is calculated as $\rho^h=\rho c_v T/c^2$, being ρ the density of the medium, T the temperature of the phonon gas and c the speed of light. Since heat conduction in dielectrics is due to the motion of the phonon gas, the continuity and momentum equations can be written as in fluid mechanics, namely,

$$\dot{\rho}^h+\rho^h_{,i}\bar{v}_i+\rho^h\bar{v}_{i_{,i}}=0, \tag{13a}$$

$$\rho^h(\dot{\bar{v}}_i+\bar{v}_j\bar{v}_{i_{,j}})=-\bar{p}_{,i}-\bar{f}_i, \tag{13b}$$

respectively. In the equations above, $\bar{v}_i$ are the components of the drift velocity of the phonons, $\bar{p}$ is the pressure of the phonon gas induced by the thermal vibration of the lattice, and $\bar{f}_i$ are the component of the frictional force per unit of volume. Equation (13b) holds since the gas is supposed to move very slowly with respect to the light. The system of Eqs. (13a) and (13b) is closed by the following set of constitutive equations:[29]

$$\bar{v}_i=\frac{q_i}{c_vT},\quad \bar{p}=\frac{\gamma\rho^h c^2}{\rho},\quad \bar{f}_i=\alpha\bar{v}_i, \tag{14}$$

being γ the Grüneisen constant and α a suitable coefficient describing the resistance to the phonon flow. From the above set of equations, it is easy matter to derive the following general heat-conduction equation:[29]

$$\tau_{\rm tm}\dot{q}_i-c_v\ell_i\dot{T}+\ell_jq_{i_{,j}}-{\rm M}_h^2\kappa T_{,i}+\kappa T_{,i}+q_i=0, \tag{15}$$

where $\tau_{\rm tm}$ is the thermomass relaxation time and ℓ_i is a suitable length parameter given by $\ell_i=\tau_{\rm tm}\bar{v}_i$. Moreover, in Eq. (15) ${\rm M}_h=q/(\rho c_vT\sqrt{2\gamma c_vT})$ stands for a dimensionless number, less than unity, which is also called thermal Mach number of the drift velocity relative to the thermal wave speed in the phonon gas.[28,29]

The last two terms of Eq. (15) correspond to Fourier law, and the first one corresponds to the heat flux relaxation time, which is analogous to the first term in Eq. (2). The second term, instead, corresponds to the relaxation of the temperature gradient, a typical term in the dual-phase-lagging constitutive equation proposed by Tzou.[5,27] The new terms are the third and fourth ones, which are nonlinear terms. In more detail, in the third term the length parameter ℓ_j depends of the heat flux itself,[29] in such a way that this term is proportional $q_jq_{i_{,j}}$ and therefore it is different from the last term in Eq. (2). We will comment it in the next paragraph. It is important to note that the mean-free path of phonons l is independent of the heat flux, and has therefore a different meaning than the vectorial length ℓ_i. Moreover, since ${\rm M}_h^2$ is proportional to the square of the heat flux, it follows that the fourth term is of the form $q^2T_{,i}$. This kind of nonlinearity does not appear explicitly in Eq. (2). However, it could appear in it if one assumes that the thermal conductivity depends on the heat flux as $\kappa_{\rm eff}=\kappa(1-{\rm M}_T^2q^2)$ with ${\rm M}_T={\rm M}_h/q$. Indeed, this kind of nonlinearity, which has been analyzed in Ref. 22, has not been considered here for the sake of simplicity.

The term in $\ell_jq_{i_{,j}}$ in Eq. (15) is a conceptually interesting term arising from the second term on the left-hand side in Eq. (13b), where it was introduced as the convective part of the material derivative of the heat flux. Indeed, in our formulation in Eq. (2), the term in $\dot{q}_j$, i.e., the time derivative of the heat flux, has some ambiguity concerning the convective term. Since the solid is at rest, one could assume that there is no convective term. However, since the phonon gas has a slow drift velocity proportional to the heat flux, given by Eq. (14), it seems logical to take this velocity in the convective term of the time derivative. Thus, we could consider that in Eq. (2) as well as in other equations we are referring to $\dot{q}_i=q_{i_{,t}}+v_jq_{i_{,j}}=q_{i_{,t}}+(q_j/\rho c_vT)q_{i_{,j}}$. In our opinion, this is the true core of the thermomass model. However, in our formalism it is not necessary to postulate a mass for the phonon fluid, although it is not against such an interpretation. In our model it is enough to take the convenient convective term in the time derivative appearing in the relaxational term. Being convective terms, they do not appear in the entropy production and they do not modify our previous analysis in Sec. III. In fact, the idea that in some situations in the analysis of heat transfer one may consider the heat flow as a hydrodynamic flow was considered by some authors as Grmela[39] and Sieniutycz[40] some years ago, although not in the context of nanosystems.

In comparison with Eq. (2), Eq. (15) is lacking the Laplacian term of the heat flux, which is a specially relevant term in phonon hydrodynamics, as it describes, for instance, how the effective thermal conductivity depends on the radius of a nanowire or the width of a thin layer.[10] Without this term, Eq. (15) would predict that the effective thermal conductivity of a nanowire would not depend on the radius, which is against the experimental observations.[6,9,10] However, it would be very easy to incorporate this kind of term in the thermomass model, by assuming that the friction term [i.e., $\bar{f}_i$ in Eq. (13b)] is not only proportional to the heat flux, but adding a second contribution proportional to the Laplacian of the heat flux. This kind of friction is of the so-called Brinkman-Navier form in usual hydrodynamics of porous media, where the friction proportional to the velocity corresponds to the Darcy law of porous media and the term in the Laplacian of the velocity is the well-known Navier-Stokes viscous friction, describing the internal friction of the fluid.

Equation (15) reduces to a Cattaneo-type equation when the second, the third and the fourth term are negligible, but with a different physical meaning of $\tau_{\rm tm}$ with respect to τ_R since $\tau_{\rm tm}$ means the lagging time from the temperature gradient to the corresponding heat flux while τ_R means the lagging time from the thermal nonequilibrium to the equilibrium state. For dielectric crystals the value of the characteristic time may differ for two orders of magnitude,[29] which results in a much slower temperature response to a heat pulse predicted by the thermomass model than that by Cattaneo's model.

The comparison with thermomass model is interesting for several reasons. In our model it is not necessary to postulate that phonons have an effective mass, or thermomass, but the generalized transport equation of the hydrodynamic form emerges naturally. Thermomass model, in its current formulation, is lacking a relevant term, namely, that of the Laplacian of the heat flux which is found in Eq. (2), but not in Eq. (15). This could be added in a natural way, and this could make the comparison between both theories more illustrative and interesting. On the other side, the thermomass structure (namely, suggesting that the equation for the heat flux may be compared to a momentum balance equation for the phonons) suggests the presence of nonlinear terms analogous to a convective contribution in the temporal derivative of the heat flux. In contrast, our identification of the coefficient μ in the nonlinear term of Eq. (2) is related to the second law and is given by Eq. (12b). But the identification of μ in Eq. (12b) is very close to the coefficient of the convective term in the thermomass model: in fact in both cases this term is proportional to the resistive time τ_R and inversely proportional to the specific heat times the absolute temperature. Indeed, the third term in Eq. (15) may be written as

$$\ell_j q_{i_{,j}} = \frac{\kappa}{2\gamma c_v (\rho c_v T)^2} q_j q_{i_{,j}} = \frac{\tau_R}{\rho c_v T} q_j q_{i_{,j}}, \tag{16}$$

since in the thermomass model $\tau_R = \kappa/(2\gamma\rho c_v^2 T)$. But this identification is close to our interpretation Eq. (12b). Further analysis is still needed, but it is clear that the comparison between our model and the thermomass model could be fruitful, provided the thermomass model in enlarged to cope with the Laplacian term in heat flux.

V. HYDRODYNAMIC ANALOGY AND STABILITY OF THE HEAT FLOW IN NANOSYSTEMS

In Sec. I we already observed that the Guyer-Krumhansl equation [Eq. (1)] does not account for nonlinear phenomena arising at a very small length scale. Therefore, in order to take into account also nonlinear effects, in Sec. III we derived Eq. (11). When the hypothesis of temperature-dependent material functions is relaxed, it becomes

$$\tau_R \dot{q}_i + q_i = -\kappa\theta_{,i} + 2\frac{\tau_R}{c_v\theta} q_k q_{k_{,i}} + l^2(q_{i_{,kk}} + 2q_{k_{,ki}}), \tag{17}$$

where we have used the relation $g = l^2/\tau_R$. It is worth noticing that, under the hypothesis of constant material functions, the equation above can be derived by combining Eqs. (3) and (5), without any approximation.[21]

Here we show its analogy with the hydrodynamic equations and point out a possible way of predicting instability of the heat flow. As we will show in this section, such an analogy can be obtained whenever q_i is negligible with respect to its spatial derivatives. Due to the small dimensions, this situation is peculiar to nanosystems, where the gradients of the heat flux are proportional to the inverse of their length.

A. Characteristic numbers

From a physical point of view, each term entering a given equation is able to model a certain effect. It is a usual practice in applied science and engineering to make approximations allowing to neglect some effects with respect to others in some given situations. However, this way of solving a problem presupposes an *a priori* choice of the approximation limits one wants to use.

In order to test the validity of a given approximation, it would be useful to characterize quantitatively the relative importance of the different effects. To this end and as one may compare only effects which are homogeneous in dimensions, it is useful to introduce some dimensionless numbers. In the next we denote by a superscript * the dimensionless unitary quantities and by a superscript r the reference quantities, i.e., the standard values of the physical quantities at which the system works.

Looking to the local balance of internal energy [Eq. (4)], we may observe that the relative importance of the left-hand side term with respect to the right-hand side one is a measure of the unsteady state of e. To understand in what conditions we may neglect the temporal rate of internal energy (namely, in what situation we are allowed to consider the problem essentially as a quasisteady-state process), taking into account the relation $de = c_v d\theta$, let us rewrite Eq. (4) as

$$\frac{c_v^r\theta^r}{t^r} c_v^* \dot{\theta}^* + \frac{q^r}{L^r} q^*_{i_{,i}} = \frac{1}{M_q}\dot{e}^* + q^*_{i_{,i}} = 0, \tag{18}$$

with

$$t^r = \frac{c_v^r L^{r2}}{\kappa^r}, \tag{19a}$$

$$M_q = \frac{q^r L^r}{\kappa^r \theta^r}. \tag{19b}$$

From Eqs. (18) and (19) one may conclude that for regular solutions of the field equations, i.e., for finite values of $\dot{e}$, it is possible to neglect the term in $\dot{e}$ whenever $M_q \gg 1$. In practical applications, one may try to interpret θ^r as the average temperature of the system, κ^r as the effective thermal conductivity of the systems at θ^r, L^r as the longitudinal length of the system, and q^r as the longitudinal heat flow due to the difference in temperature through the ends of the system.

Forcing the fluid dynamic nomenclature, let us refer to the dimensionless number in Eq. (19b) as the Mach number for the heat flow. Indeed, this fanciful identification, as well as those we will make in the next, stems from the observation that the form of the constitutive equation for the heat flux in phonon hydrodynamics is analogous to the hydrodynamic equation for the velocity of a viscous fluid, with q_i playing the role of the fluid speed v_i, $\theta_{,i}$ the role of the pressure gradient $\mathcal{P}_{,i}$, and l^2/κ the role of viscosity. This latter identification may be easily seen from the linearized steady-state version of Eq. (17), which reduces to $l^2 q_{i_{,kk}} = \kappa\theta_{,i}$ and compare this with the linearized steady-state version of the Navier-Stokes equations. Note that here we are not making an identification, but only an analogy, which is useful in linear and steady-state situations. However, when relaxational and nonlinear terms are also included a new question arises concerning the analogous of the mass density in the Navier-Stokes equation. This was precisely one of the motivations of the thermomass model of heat transport analyzed in Sec. IV.

The Mach number in Eq. (19b) may be also written as the ratio of the reference heat flux q^r divided by Q^r, being $Q^r=\kappa^r\theta^r/L^r$. In the particular case that L^r, instead of being taken as the length of the system, was taken as $L^r=q\kappa/[2\gamma c_v(\rho c_v T)^2]$, the Mach number for the heat flux in Eq. (19b) coincides with the square of thermal Mach number in Eq. (15).

Taking into account the relations between the thermal quantities and the hydrodynamic ones, it is possible to observe that, as in fluid dynamics the Mach number (M) is given by the ratio between the body speed and the speed of sound (assumed with a suitable reference speed), in our model M_q is given by the ratio between the actual heat flux in the system at hand (i.e., q^r) and a reference heat flux (i.e., $\kappa^r\theta^r/L^r$). Moreover, as in fluid dynamics M represents the percent rate, per unit time, of the mass density along a given particle stream line (and therefore it is a measure of the compressibility of the fluid), here M_q will be used as a measure the temporal rate of e.

From the practical point of view one may try to check a critical value of M_q representing the threshold between the steady-state problem and an unsteady one. Experimental situations could complement and test the validity of this theoretical proposal. However, let us underline that the possibility of interpreting a characteristic number as a measure of the relative importance of an effect with respect to one another (and all the arising consequences) is always conditioned by the appropriate choice of the reference quantities.

Let us concentrate our attention now on Eq. (17), describing the evolution of the heat flux. According with the conclusion above, when $M_q \gg 1$ we may assume that the heat flux is a solenoidal vector. In this case Eq. (17) can be rewritten as

$$\frac{q^r}{t^r}\dot{q}_i^* + \frac{q^r}{\tau_R^r}\frac{q_i^*}{\tau_R^*} - \frac{2}{c_v^r\theta^r}\frac{q^{r2}}{L^r}\frac{1}{c_v^*\theta^*}q_k^*q_{k,i}^* - \frac{l^{r2}}{\tau_R^r}\frac{q^r}{L^{r2}}\frac{l^{*2}}{\tau_R^*}q_{i,kk}^* + \frac{\kappa^r}{\tau_R^r}\frac{\theta^r}{L^r}\frac{\kappa^*}{\tau_R^*}\theta_{,i}^* = \frac{1}{\mathrm{St}_q}\dot{q}_i^* + \tau_R^r\frac{\mathrm{Re}_q}{\mathrm{Kn}_q^2}\frac{q_i^*}{\tau_R^*} - \frac{1}{c_v^*\theta^*}q_k^*q_{k,i}^* - \frac{1}{\mathrm{Re}_q}\frac{l^{*2}}{\tau_R^*}q_{i,kk}^* + \frac{1}{\mathrm{Fr}_q}\frac{\kappa^*}{\tau_R^*}\theta_{,i}^* = 0, \tag{20}$$

wherein we have introduced the following quantities:

$$\mathrm{St}_q = 2\frac{q^r t^r}{c_v^r\theta^r L^r}, \tag{21a}$$

$$\mathrm{Re}_q = 2\frac{q^r\tau_R^r L^r}{l^{r2}c_v^r\theta^r}, \tag{21b}$$

$$\mathrm{Kn}_q = \frac{l^r}{L^r}, \tag{21c}$$

$$\mathrm{Fr}_q = M_q\,\mathrm{Re}_q\,\mathrm{Kn}_q^2 = 2\frac{q^{r2}\tau_R^r}{\kappa^r c_v^r\theta^{r2}}, \tag{21d}$$

which, along with the same observations as above, we call, respectively, thermal Strouhal number, thermal Reynolds number, thermal Knudsen number, and thermal Froude number. Under the same identifications as before for the reference quantities, it is also possible to identify c_v^r, l^r and τ_R^r, respectively, as the specific heat of the system, the mean-free path of phonons, and the resistive relaxation time at the average temperature θ^r. The reference time t^r used in Eq. (20), in principle, would be different from that used in Eq. (18). However, if one uses the reference time defined in Eq. (19a), from Eq. (21a) it follows that $\mathrm{St}_q=2M_q$.

Equation (20) points out that it is possible to neglect the heat flux with respect to the spatial variations in the heat flux itself whenever $\tau_R^r\,\mathrm{Re}_q/\mathrm{Kn}_q^2 \ll 1$. As we said above, this condition is fulfilled frequently in nanosystems.[21] In this case Eq. (20) becomes

$$\tau_R\dot{q}_i - 2\frac{\tau_R}{c_v\theta}q_k q_{k,i} = -\kappa\theta_{,i} + l^2 q_{i,kk}, \tag{22}$$

which is very similar to the Navier-Stokes equation describing the motion of an incompressible viscous fluid in the absence of external force and gives a better understanding of the strict relation between the hydrodynamic quantities and the thermal ones. Note that in Eq. (22) the nonlinear contribution is related to $q_k q_{k,i}$, while in the Navier-Stokes equation it has the form $v_k v_{i,k}$.

Equation (22) allows to relate the term in $\tau_R/(c_v\theta)q_k q_{k,i}$ with the convection phenomena in the evolution of the heat flux, the term in $l^2 q_{i,kk}$ with the irreversible diffusion phenomena, and the term in $\kappa\theta_{,i}$ with the driving force due to inhomogeneities in the thermal field. Note that the possibility of having both a convective contribution and a diffusive one must not be surprising. In fact, in the framework of extended irreversible thermodynamics[1] the heat flux has its own evolution equation, namely,

$$\dot{q}_i = -\frac{q_i + \kappa\theta_{,i}}{\tau_R} + \frac{1}{\tau_R}Q_{ik,k}, \tag{23}$$

being Q_{ik} a second-order tensor representing the flux of heat flux per unit time. Therefore, according to the definition of flux itself, one may split Q_{ik} in the convective part and in the diffusive part. This way we may conclude that, in the context of phonon hydrodynamics, in Eq. (17) the thermal Strouhal number [Eq. (21a)] gives information about the relative importance of unsteady phenomena with respect to the convection phenomena, whereas the thermal Froude number [Eq. (21d)] accounts for the relative importance of the convection phenomena with respect to the driving force due to inhomogeneities in the thermal field. This is in analogy with the physical meanings of hydrodynamic Strouhal number (St) and hydrodynamic Froude number (Fr). These are further reasons of the nomenclatures we used for Eqs. (21a) and (21d). Note that, in contrast with the formal analogy between the definition of the thermal Mach number [Eq. (19b)] and that of the hydrodynamic Mach number we observed above, in classical hydrodynamics St and Fr have definitions which are not formally the same of those in Eqs. (21a) and (21d), although they play an analogous role. Remember that in hydrodynamics one has $\mathrm{St}=t^r v^r/L^r$, and $\mathrm{Fr}=v^{r2}/(L^r\bar{g}^r)$, being v^r the reference fluid speed and $\bar{g}^r$ a reference acceleration, which is usually taken as the gravity acceleration, but $q^r/c_v^r\theta^r$ has dimensions of a speed, i.e., units of m/s.

The thermal Reynolds number [Eq. (21b)] points out, instead, the relative importance of convection with respect to the irreversible diffusion. Its definition is similar to the definition of hydrodynamic Reynolds number (Re), i.e., $\mathrm{Re}=v^rL^r/\nu^r$, being ν^r the reference kinematics viscosity. That way we may assume that in phonon hydrodynamics the ratio $2\tau_R/(l^2c_v\theta)$ plays the same role of ν in hydrodynamics. Further information about the relative importance between other effects may be enlightened by obtaining suitable ratio between these characteristic numbers.

B. Stability of the heat flow: A simple example

Let us now illustrate by a simple example the possibility of relating the stability of heat flow with the value of some thermal numbers. To this end, let us suppose $M_q \gg 1$ and $\mathrm{Re}_q \ll \mathrm{Kn}_q^2/\tau_R^r$. From Eqs. (4) and (17) we have

$$q_{i_{,i}}=0, \tag{24a}$$

$$\dot{q}_i-\mu q_k q_{k_{,i}}-\eta q_{i_{,kk}}+\pi_{,i}=0, \tag{24b}$$

being $\mu=2/(c_v\theta)$, $\eta=l^2/\tau_R$, and $\pi=\kappa\theta/\tau_R$. Prescribe then the following boundary values:

$$q_i(x_j;t)=q_i^b(x_j;t), \quad \forall\, x_j\in\partial\Omega, \quad \forall\, t\geq 0 \tag{25}$$

as the initial ones

$$q_i(x_j;0)=q_i^0(x_j), \quad \forall\, x_j\in\Omega, \tag{26}$$

where $q^0_{i_{,i}}(x_j)=0$, $\forall x_j\in\Omega$, being Ω the spatial domain occupied by the nanowire, and $\partial\Omega$ the boundary of the system, respectively. Note that both $\partial\Omega$ and Ω cannot change in time, since we are regarding the nanosystem as a rigid body. It is worth observing that Eq. (24a) is not able to furnish now the function e and hence, we cannot calculate the function θ appearing in the right-hand side of Eq. (24b) from its constitutive equation. As a consequence, θ must be regarded now as an additional unknown quantity, as the components of the heat flux. The four unknowns e and q_i are to be calculated by solving the system in Eqs. (24). The same situation holds in classical hydrodynamics where, in the presence of the constraint of incompressibility, the pressure cannot be calculated through a constitutive equation, but becomes an additional unknown quantity.

The solutions of the initial boundary value problem (IBVP) in Eqs. (24a), (24b), (25), and (26) will be denoted as

$$\{q_i(x_j;t;q_i^0);\pi(x_j;t;q_i^0)\}. \tag{27}$$

We aim to study the stability of these solutions when the initial values $q_i^0(x_j)$ are perturbed. Thus, let us consider the further solution

$$\{q_i^a;\pi^a\}=\{q_i(x_j;t;q_i^0+\delta q_i^0);\pi(x_j;t;q_i^0+\delta q_i^0)\}, \tag{28}$$

which still satisfies Eqs. (24) and (25), but differs from the initial value $\{q_i(x_j;t;q_i^0);\pi(x_j;t;q_i^0+q_i^0)\}$ since

$$q_i^a(x_j;0)=q_i(x_j;0;q_i^0+\delta q_i^0)=q_i^0(x_j)+\delta q_i^0(x_j). \tag{29}$$

If the solutions (27) and (28) behave in the same way for increasing time, we face with stable solutions, otherwise we have instable solutions. To be more explicit, we are interested in determining whether the form which the fields in Eq. (27) take as $t\to\infty$ is stable with respect to perturbations in the initial conditions. This problem can be analyzed by introducing the following IBVP:

$$\delta q_{i_{,i}}=0, \tag{30a}$$

$$\delta\dot{q}_i-\mu(q_k\delta q_{k_{,i}}+\delta q_k q_{k_{,i}}+\delta q_k\delta q_{k_{,i}})-\eta\delta q_{i_{,kk}}+p_{,i}=0, \tag{30b}$$

$$\delta q_i(x_j;t)=0, \quad \forall\, x_j\in\partial\Omega, \quad \forall\, t\geq 0, \tag{30c}$$

$$\delta q_i(x_j;0)=\delta q_i^0(x_j), \quad \forall\, x_j\in\Omega, \tag{30d}$$

which governs the evolution of the disturbance $\{\delta q_i;p\}=\{q_i^a-q_i;\pi^a-\pi\}$. That way, the stability we are looking for coincides with the stability of the problem in Eqs. (30).[41] If we define the average energy of a disturbance as

$$\mathcal{E}(t)=\frac{1}{\mathcal{M}(\Omega)}\int_\Omega|\delta q_i|^2 d\Omega, \tag{31}$$

being $\mathcal{M}(\Omega)$ the measure of the volume of Ω, we may call the solution of Eqs. (30) stable to the initial perturbations if[41]

$$\lim_{t\to\infty}\frac{\mathcal{E}(t)}{\mathcal{E}(0)}=0. \tag{32}$$

In order to apply to a very simple situation this stability criterion, let us suppose that the disturbances are characterized by a small amplitude, so that we have $\delta h/h\ll 1$, being h the generic unperturbed quantity. Without loss of generality, this allows us to disregard nonlinear third-order terms in the perturbations, too. Finally, just for the sake of simplicity, suppose also $\mathrm{St}_q\gg 1$. Along with previous observations, in this case we have $\delta\dot{q}_i=0$, and Eq. (30b) becomes

$$\mu[\delta(q_k q_{k_{,i}})+\delta q_k\delta q_{k_{,i}}]=p_{,i}-\eta\delta q_{i_{,kk}}-\delta\mu q_k q_{k_{,i}}, \tag{33}$$

which, having present the hypothesis $\delta h/h\ll 1$, up to the second-order in the perturbations, yields

$$|\delta q_i|^2=\frac{1}{\mu^2|q_{k_{,i}}|^2}|\eta\delta q_{i_{,kk}}-p_{,i}|^2. \tag{34}$$

Therefore, if $M_q\gg 1$ and $\mathrm{Re}_q\ll \mathrm{Kn}_q^2/\tau_R^r$, the heat flow remains stable under initial perturbations if

$$\lim_{t\to\infty}\frac{\displaystyle\int_\Omega\left(\frac{c_v\theta}{2\tau_R}\right)^2\left(\frac{|l^2\delta q_{i_{,kk}}-\kappa\delta\theta_{,i}|}{|q_{i_{,k}}|}\right)^2 d\Omega}{\displaystyle\int_\Omega \delta q_i^0 d\Omega}=0, \tag{35}$$

once we have used previous identifications for μ, η, and π.

For finite values of $\mathcal{E}(0)$, from Eq. (35) we may conclude that, if the gradient of the heat flux does not tend to zero as

$t \to \infty$, the stability of q_i will be recovered if the perturbations in the initial values are such that $l^2 \delta q_{i,kk} \to \kappa \delta \theta_{,i}$ for increasing time. More generally, it is sufficient that the perturbations in the initial values are such that the integral in the numerator of the left-hand side of Eq. (35) is infinitesimal.

The physical interpretation of the result above is the following. For constant internal energy, the gradient of **q** can be interpreted as the thermodynamic force which drives the heat flow along a given direction. In Eq. (35) the strength of such a force is represented by the term $q^2_{i,k}$. On the other hand, the strength of the sole initial perturbation appearing in Eq. (35) is represented by the quantity $l^2 \delta q_{i,kk} - \kappa \delta \theta_{,i}$. For large t, if the initial perturbation has order of magnitude which is smaller than that of the driving force, then it will be not capable of changing appreciably the direction of $\boldsymbol{q}$, so that the heat flow remains stable.

On the other hand, if for large t the order of magnitude of the initial perturbation gets high values enough to render finite the integral above, i.e., if it is higher than that of the driving force, hence the perturbation can deviate the heat flux from the direction previously determined by the initial conditions, inducing so disordered and unpredictable evolutions of the flow, as, for instance, turbulence and vorticity.

Finally, let us observe that, since the form of the domain is known, the integral above can be estimated,[41] obtaining so a threshold for the initial perturbation at which the turbulent regime arises. Such a threshold can be useful in calculating the risk of thermal damage in Micro/Nano Electro Mechanical Sensors design.

VI. CONCLUSIONS

In the present paper we have proposed a model of rigid heat conductor with a scalar internal state variable, in which the evolution of the heat flux is ruled by a nonlinear Guyer-Krumhansl equation. The internal variable can be interpreted as a dynamical nonequilibrium temperature. A proportionality law of Fourier type between heat flux and dynamical temperature has been postulated. Under the hypothesis of temperature-dependent thermophysical quantities, we verified that the model is compatible with thermodynamics and derived a nonlinear extension of the classical Guyer-Krumhansl equation. Such an equation can offer a valid tool in the study of heat conduction in nanosystems, where nonlinear effects become important and cannot be described by the linear Guyer-Krumhansl equation.

After introducing some dimensionless numbers, which are suitable to express the relative importance of some of the quantities entering the system of equations with respect to other ones, we have proved in a simple case the stability of the heat flow under a perturbation in the initial conditions. To this end, we have exploited the analogy of our system of equations with that of classical hydrodynamics of viscous incompressible fluids. Although we have considered a very special and simple case, the procedure is related to important concepts, namely, the analogy with hydrodynamics and the possibility of applying the results of the theory of stability of fluid motions. More complex situations as well as specific explicit applications will be considered in future researches.

Furthermore, we have compared the evolution equation for the heat flux obtained in the present model with that proposed in the thermomass model.[28–30] It seems that a confluence of both approaches is feasible and would lead to a wide-encompassing description of heat transport in nanosystems. In particular, we have commented that the nonlinear terms appearing in the thermomass model come from a convective contribution to the time derivative of the heat flux. This convective contribution seems logical and it may be also incorporated in our model in a natural way. But our model has another nonlinear contribution [the last term in Eq. (2)], which comes from nonlinear terms in a constitutive equation, and not from a convective term. Therefore, this contribution is restricted by the second law of thermodynamics. Though here we have emphasized the transport equations for the bulk heat flux, it should not be forgotten that the slip heat flow along the walls may also play a very relevant role in the description of heat transport in nanowires,[42] and therefore it must be taken into consideration in a general analysis of the problem. It would be of interest to explore how such a slip-wall heat flux could influence the stability analysis undertaken in Sec. V B, where a nonslip flow has been assumed, in analogy with usual hydrodynamics.

For the sake of completeness, let us compare our results with those obtained in the super-Burnett expansion of kinetic theory. In Sec. V we noticed that, in the hypothesis of constant material functions, Eq. (17) either follows from Eqs. (3) and (5), without need of disregarding higher-order terms, or it replaces Eq. (11) once in its derivation third-order terms are neglected. Let us observe that it is considerably different from equations obtained in the super-Burnett expansion of kinetic theory. In such a framework, a transport equation for the heat flux up to third order was obtained by Cha and McCoy.[43] The full equations consist of more than 40 terms, including couplings between gradients of temperature, velocity, and density. In a quiescent system with homogeneous density and in the steady state, such equation reduces to

$$q_i = -\kappa \theta_{,i} - a\theta_{,kk}\theta_{,i} - b\theta_{,ik}\theta_{,k} - c\theta_{,i}\theta_{,k}\theta_{,k} - d\theta_{,kki}, \quad (36)$$

with a, b, c, and d phenomenological parameters, whose numerical value may be obtained from kinetic theory for different kinds of interaction potentials. In contrast with Eq. (17), this equation does not contain time derivatives of the heat flux and its formal structure is expressed in terms of the temperature gradient rather than in gradients of the heat flux itself. Even when q_i is approximated in Eq. (17) up to first order as $q_i \approx -\kappa \theta_{,i}$, the ensuing equation is still different from Eq. (17). The differences are still higher for unsteady fast-varying situations, which are situations were instability may most probably arise. Therefore, the topic of nonlinear and nonlocal constitutive equations is very rich for exploration.

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